Turbulent Spray Atomization Model for Diesel Engine Simulations

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Project ID: ACS105

Overview Slide

Timeline

- **Start date:** Jan 18, 2016
- **End date:** Jan 17, 2019
- **Percent complete:** 35%

Budget

- **Total project funding**
  - DOE share: $745k
  - GT cost share: $84k (10%)
- **Funding received in FY2016**
  - GT: $164k
  - ANL: $84k
- **Funding for FY2017**
  - GT: $163k
  - ANL: $84k

Barriers Addressed

- Lack of fundamental knowledge of advanced engine combustion regimes (A)
- Lack of modeling capability for combustion and emission control (C)
- Cost (G)

Partners

Overall Project and FY2016 Objectives

Project Objectives

- Formulate **new multi-physics Lagrangian spray atomization model** that accurately predicts **spray morphology** and air-fuel preparation under advanced diesel combustion regimes.
  - High and low ambient densities
  - Fuels with properties dissimilar to petroleum diesel
- Generate a **comprehensive quantitative spray measurement dataset** for spray model validation.
  - Spatially-resolved spray morphology over a wide range of operating conditions
- **Improved understanding** of physics governing atomization in diesel fuel sprays.

Inaccuracies in model physics masked by tuning and lack of quantitative morphology data
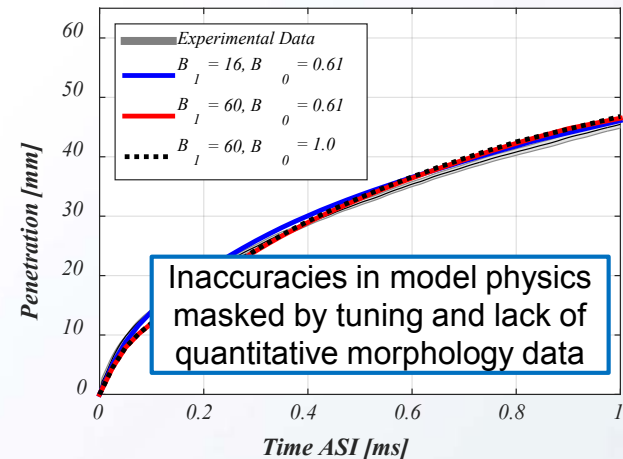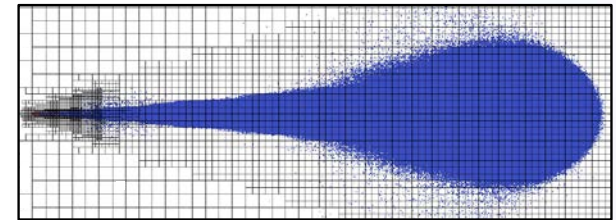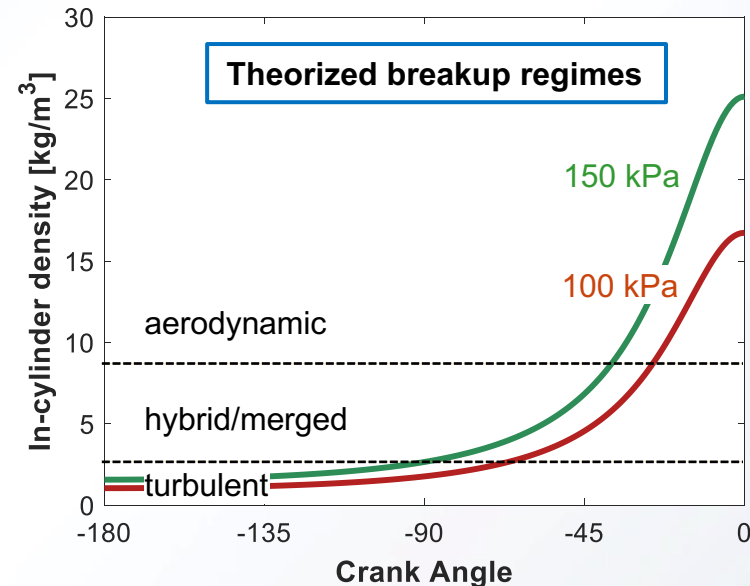
FY2016 Objectives

- Develop/Demonstrate two **new spray diagnostics** to quantify spray morphology.
- Implement **benchmark Lagrangian spray breakup models** into OpenFOAM and perform initial model performance assessment.

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Project Impact

A. Lack of fundamental knowledge of advanced engine combustion regimes

- Sprays inherent to fuel-air preparation in all direct-injection engines
- Mechanisms of fuel spray atomization unknown
- DI fuel sprays will see a wide range of environmental conditions under advanced combustion regimes

Theorized breakup regimes

150 kPa

100 kPa

aerodynamic

hybrid/merged

turbulent

In-cylinder density [kg/m^3]

Crank Angle

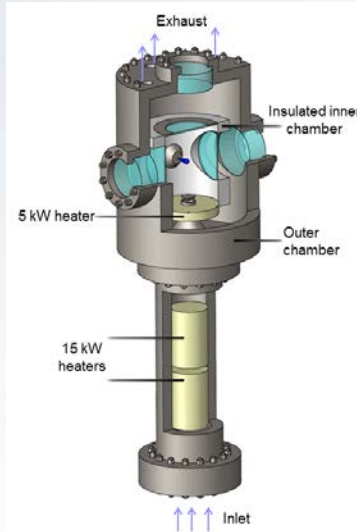## C. Lack of modeling capability for combustion and emission control

- Spray models are critical to predictive DI engine simulation
- Existing spray models developed/validated primarily for conventional diesel combustion regimes (aerodynamically-driven atomization assumed)

G. Cost

- Predictive engine simulation will advance LTC and reduce aftertreatment cost.

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Project Resources

GT High Pressure and Temperature Continuous Flow Chamber
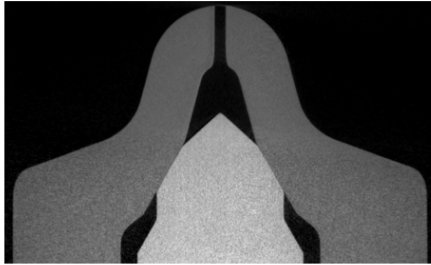

Argonne Advanced Photon Source

GT FoRCE Cluster

Contribution-based institute-managed HPC cluster

8000 shared cores

Overall Technical Approach

New Diagnostics for Quantitative Spray Morphology Measurements

Improved Fundamental Understanding of Atomization Physics

New Multi-Physics Lagrangian Spray Atomization Model

- Address lack of quantitative data for spray model development and validation.
- Development of new scattering-absorption measurement ratio (SAMR) technique to quantify 2D and 3D spray morphology (liquid volume fraction and SMD distribution) in practical diesel sprays.

BP1	BP2	BP3
Turbulent liquid jet atomization	Aerodynamic forces	Unconventional liquid properties

Increasing physical complexity

- Wide range of experimental conditions probed quantitatively for the first time.
- $\rho_{ambient}$, P_{inj}, d_{nozzle} used to control turbulent and aerodynamic forces within experiments.
- Leverage improved fundamental understanding to guide development of new open-source Lagrangian spray model in OpenFOAM.
- Target predictive performance over wide range of advanced combustion operating conditions.

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Collaboration and Coordination with Other Institutions

Georgia Institute of Technology

Physical Model(s) with Accurate Representation of Spray Breakup Physics

High-Fidelity Validation Data X-Ray + Visible Light Spray Diagnostics

Engine Combustion Network

- Well characterized injector nozzles
- Over 40 international participants from universities, national labs, and industry
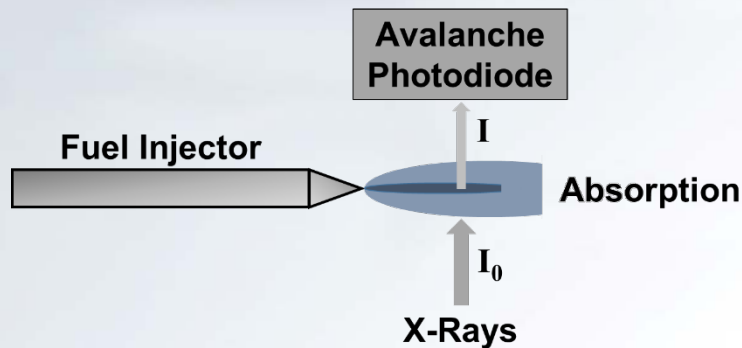- Validation data and modeling results will be contributed to ECN database

Argonne NATIONAL LABORATORY

	2016	2017	2018
Generate Validation Data Turbulent Breakup Conditions (low ρ_{amb})	◇ ◇ ◇ ◆(green)		
Develop Turbulent Atomization Submodel	◆	◇ ◇	
Generate Validation Data Aerodynamic Breakup Environments (high ρ_{amb})		◇ ◆(red)	
Extend Model Formulation			◇ ◇
Generate Validation Data Unconventional Fuel Properties			◇
Validation of Hybrid Atomization Model			◇

✓ **April 2016:** Measurement set-up and determine symmetry of Spray D

✓ **July 2016:** Radiography measurements at APS

✓ **October 2016:** USAXS measurement at APS

✓ **January 2017:** Implementation/Validation of benchmark spray models

✓ **BP1 Go/No-Go:** Demonstrate 2-D spray morphology measurement

▪ **April 2017:** Evaluate response of benchmark models and determine model improvement path

X-Ray Radiography (Argonne)

$$\frac{I}{I_0} = e^{-\left(\frac{\mu}{\rho}\right)PD}$$
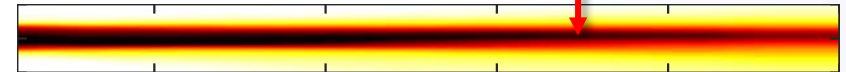
Position [mm]

Diffuse Back Ilumination Extinction Imaging (GA Tech)

Fresnel lens
D=170 mm
f=152 mm

LED with collimator

Fuel Spray

140 mm   152 mm

250 mm

Fuel Injector

Avalanche Photodiode

I

Absorption

I_0

X-Rays

High-speed
CMOS camera
f/1.2 50 mm
visible lens

Engineered
diffuser
D=100 mm
θ=15°

Engineered
diffuser
D=25 mm
θ=20°

$$\frac{I}{I_o} = e^{-\tau}$$

Distance from nozzle [mm]

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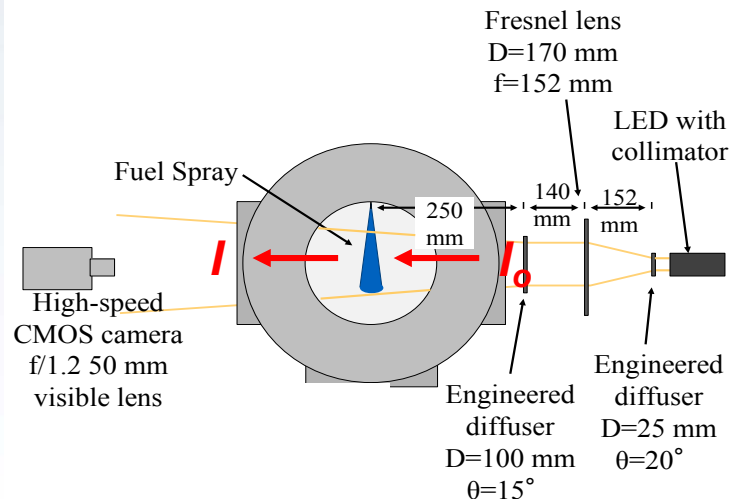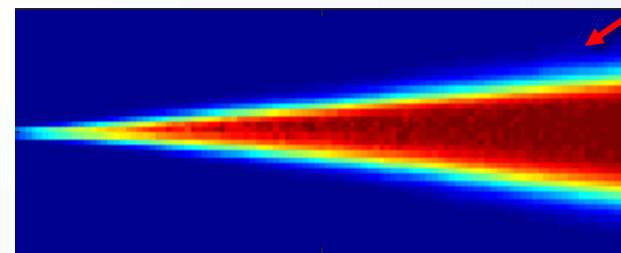
Suite of radiography measurements completed at low ambient densities - focus on turbulent breakup conditions

- X-ray radiography measures projected liquid mass
  - Liquid volume fraction at isothermal conditions

- Measurements at 6 non-vaporizing operating conditions completed for Spray D (dodecane)
  - $\rho_{ambient}$: 1.2, 2.4, 22.8 kg/m^3
  - $P_{injection}$: 50, 150 MPa

- Each data point is ensemble average of 16-32 measurements

- Measurements from two different viewing angles demonstrate good symmetry of Spray D mass distribution (nozzle #209133)

0° view
80° view
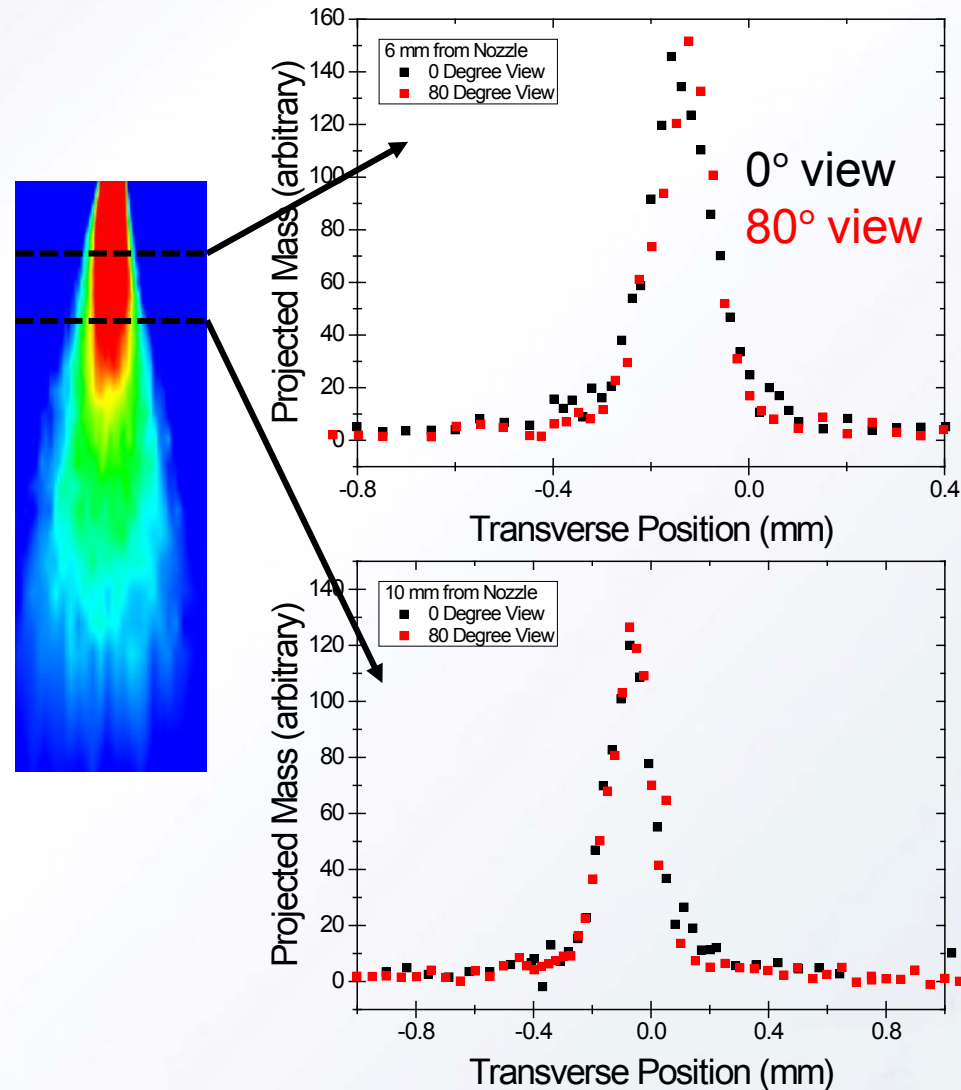
USAXS measurement demonstrate spray morphology measurement along optically thick spray centerline

Small Angle X-Ray Scattering (SAXS)
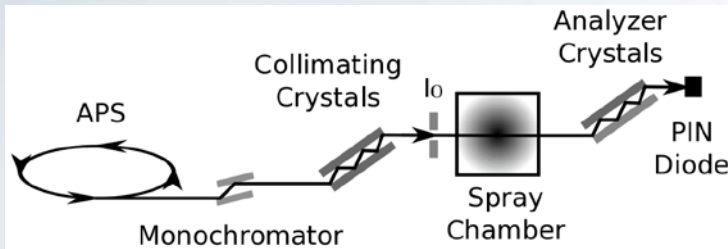
- Measure number of x-rays scattered as a function of angle
- Absolute magnitude of the scattering depends on the *surface area* of the scatterers
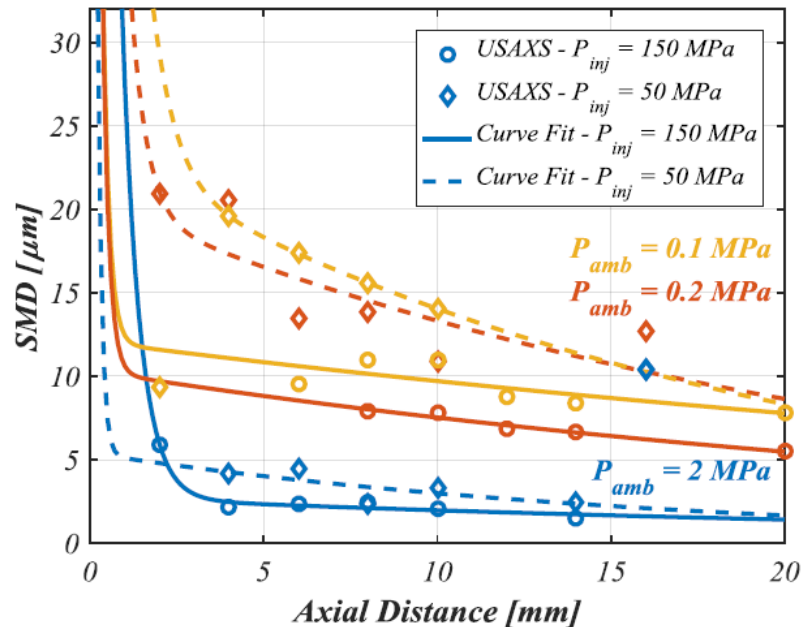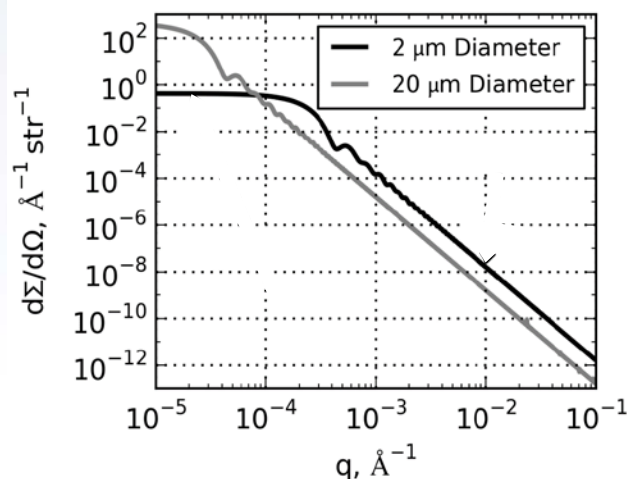
Large scale trends behave as expected:

- Measured SMD decreases with increasing $\rho_{ambient}$
- Measured SMD decreases with increasing P_{inj}
- SMD is more sensitive to P_{inj} at low ambient densities (turbulent breakup conditions)

New diagnostic for spatially resolved measurement of diesel spray morphology: Scattering-Absorption Measurement Ratio (SAMR)
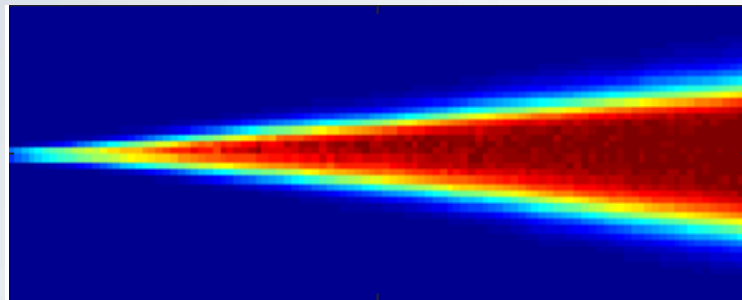
Distance from nozzle [mm]

$\tau \; [-]$

$$\frac{I}{I_o} = e^{-\tau}$$

$$\tau = \int_{-\infty}^{+\infty} \overline{C_{ext}} N \, dz$$

$$\tau = \int_{-\infty}^{+\infty} \frac{\overline{C_{ext}LVF}}{(\pi/6)\overline{\overline{d^3}}} \, dz$$

$C_{ext} = f(d,\lambda,n)$ is the scattering cross-section and is determined by Mie-scatter theory (see back-up slides)

Light extinction due to droplet scattering is proportional to path-integrated **droplet number density (N)** or **liquid volume fraction (LVF)** and mean **drop size (d)**.

Second measurement needed to solve inverse problem → x-ray radiography (absorption measurement of projected density)

τ / PD measurement ratio is proportional to the path-integrated SMD

$$\tau = \int_{-\infty}^{+\infty} \frac{\overline{C_{ext}}LVF}{(\pi/6)\overline{d^3}} dz$$

$$PD/\rho = \int_{-\infty}^{+\infty} LVF dz$$

$$\frac{\tau}{PD} \propto \frac{\overline{C_{ext}}}{\overline{d^3}} \propto \frac{1}{SMD}$$

- MiePlot used to calculate scattering cross-section C_{ext} (backup slide)
- Rayleigh-scattering limit solution is non-physical (SMD < 0.1 μm)
- Mie-scattering solution is insensitive to assumed drop-size distribution along light path.

10-mm axial location

1.2 kg/m^3, 300 K
P_{inj} = 500 bar

$\tau = 2.0$

1 μg/mm^2
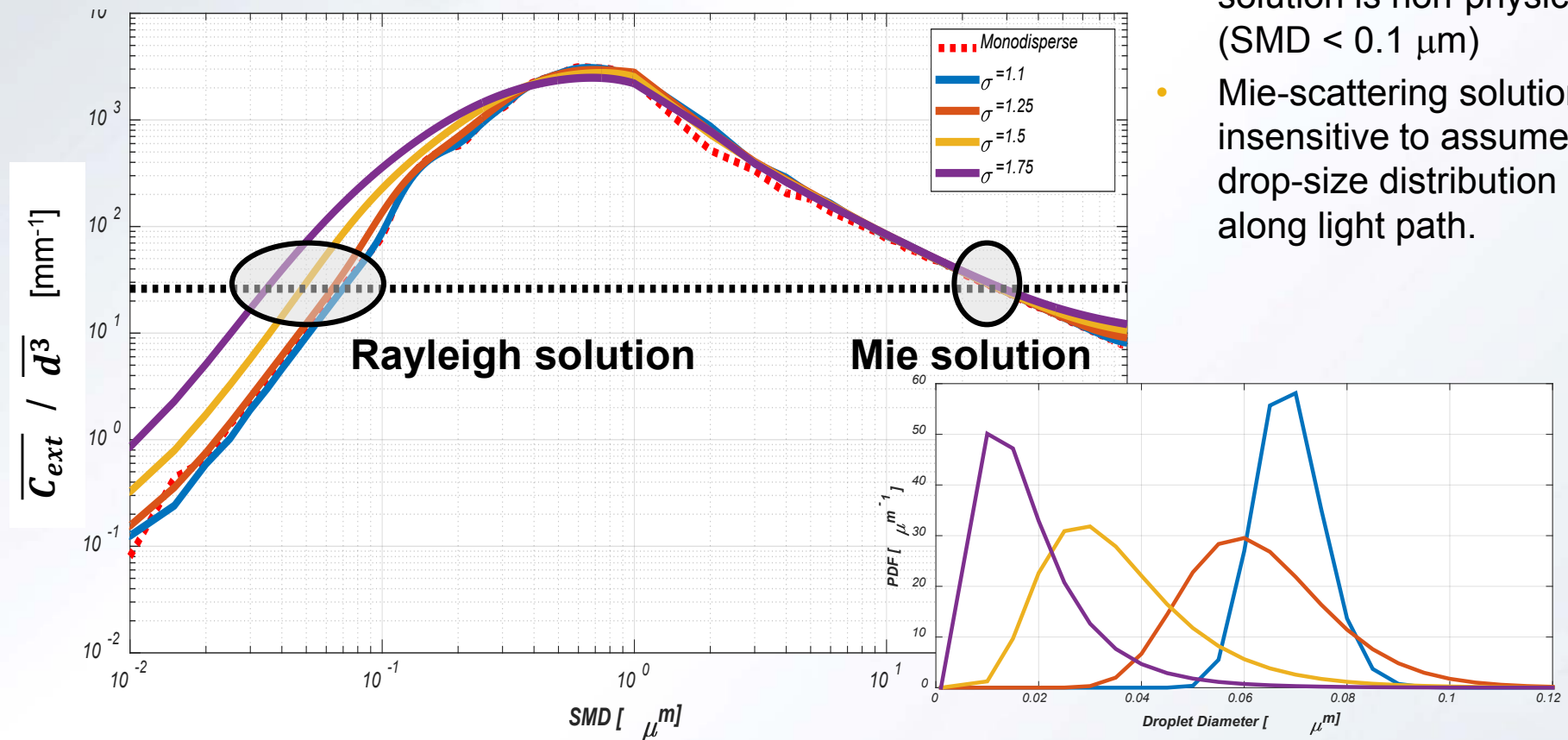
- Optical thickness (τ) and radiography (PD) measurements have different measurement sensitivities at the radial extents of the spray.

- Critical issue: Radiography signal is below noise floor throughout much of the spray periphery.
  - Contrast agent not used in these experiments

- Mie-scattering assumptions invalid when multiple scattering effects present ($\tau > 1.0$)
  - Error is low for small droplets and narrow collection angle for $\tau > 2.0$

- Viable SAMR measurement lies between these limits.

- Critical issue: spray asymmetries are more prominent in these regions.

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BP1 Go/No-Go: Scattering-Absorption Measurement Ratio (SAMR) successfully demonstrated for Spray D

10-mm axial location

1.2 kg/m^3, 300 K
P_{inj} = 500 bar

$\tau \sim 2.0$
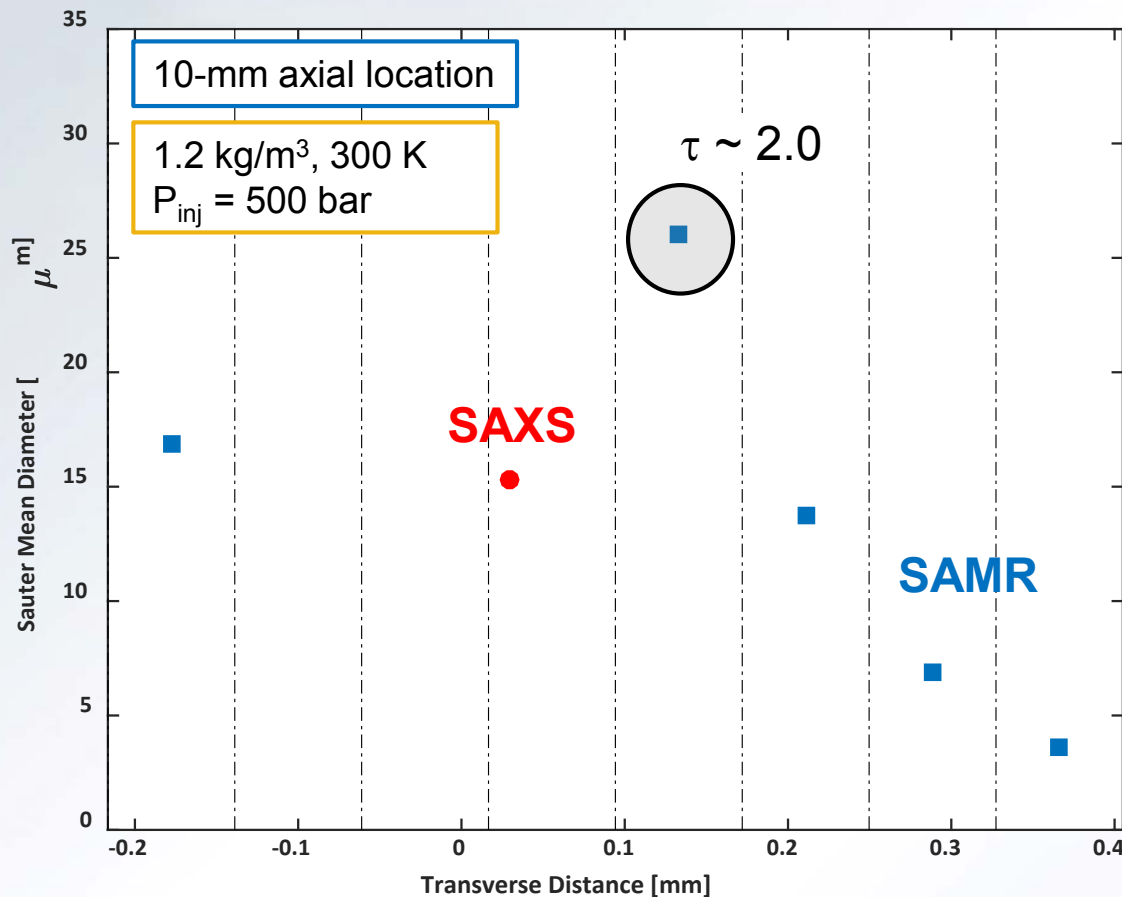
SAXS

SAMR

- Initial SMDs quantified by SAMR are physically consistent with SAXS measurements at spray centerline.
  - Larger uncertainties for measurement points closest to centerline (2.0 < τ < 1.0)
- Processing of data into 2D maps of LVF and SMD ongoing.
- Tomographic reconstruction with multiple viewing angles can be used to generate 3D maps.
- Time-resolved measurements also achievable to quantify breakup transients.
- **Critical Issue: Uncertainties need to be quantified and minimized:**
  1. τ / PD measurement alignment
  2. Multiple scattering errors

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Benchmark spray models implemented in OpenFOAM
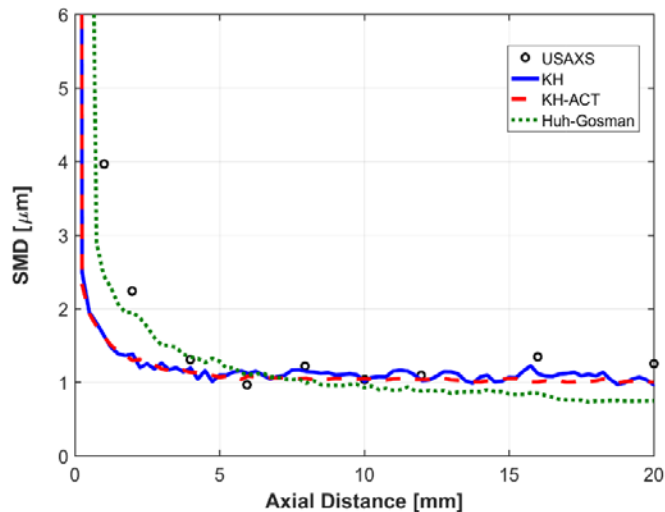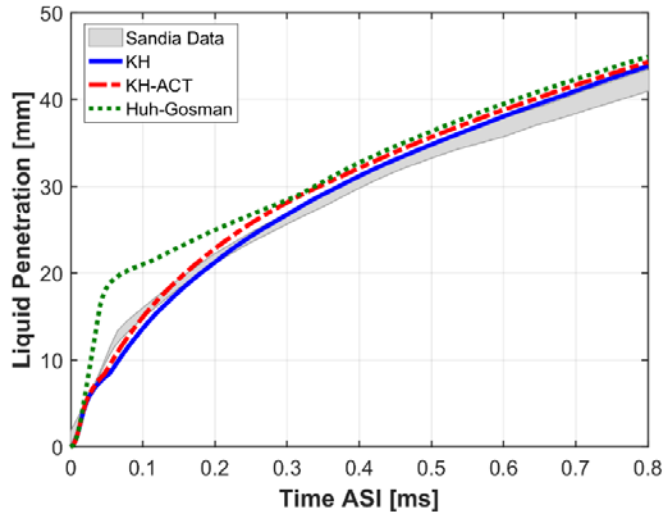
- Three benchmark Lagrangian primary breakup models:
  - <u>KH:</u> Aerodynamically driven interface instabilities lead to droplet formation
  - <u>Huh-Gosman:</u> Liquid turbulence properties drive interface instabilities and droplet formation
  - <u>KH-ACT:</u> Hybrid model incorporating aerodynamic and liquid turbulence mechanisms

- Verified grid and lagrangrian parcel count convergence.
- Calibrated models to ECN Spray A.
- Evaluation of benchmark model response against BP1 data currently ongoing.
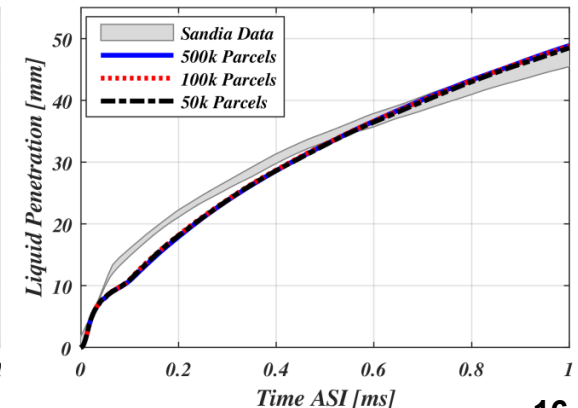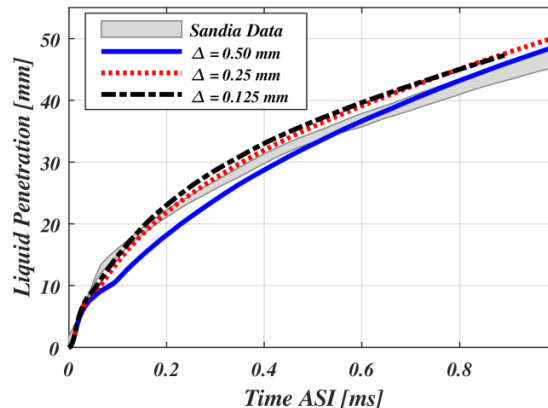
Model sensitivities indicate need to further evaluate appropriate turbulent breakup physics at low ambient densities

- KH model matches experimental sensitivities at high $\rho_{ambient}$ conditions (not shown).

- KH and KH-ACT models demonstrate similar response to changes in $\rho_{ambient}$, P_{inj} and d_{nozzle}
  - Aerodynamic breakup favored in these models under all conditions
  - KH-ACT does not appear to transition to turbulence dominated breakup at any modeled conditions
  - SMD insensitive to $\rho_{ambient}$ for $\hat{\rho} \geq 300$

- New model scaling for turbulent breakup introduced based on experimental work of Faeth group (KH-Faeth)

- KH-Faeth model predicts different physical sensitivities, especially at low $\rho_{ambient}$
  - For a given d_{nozz}, SMD ↓ with increasing P_{inj} at all conditions (consistent with measurements)
  - SMD responsive to $\rho_{ambient}$ for $\hat{\rho} \geq 300$

- Further quantitative evaluation against BP1 data is needed to determine appropriate turbulent breakup scaling (ongoing)

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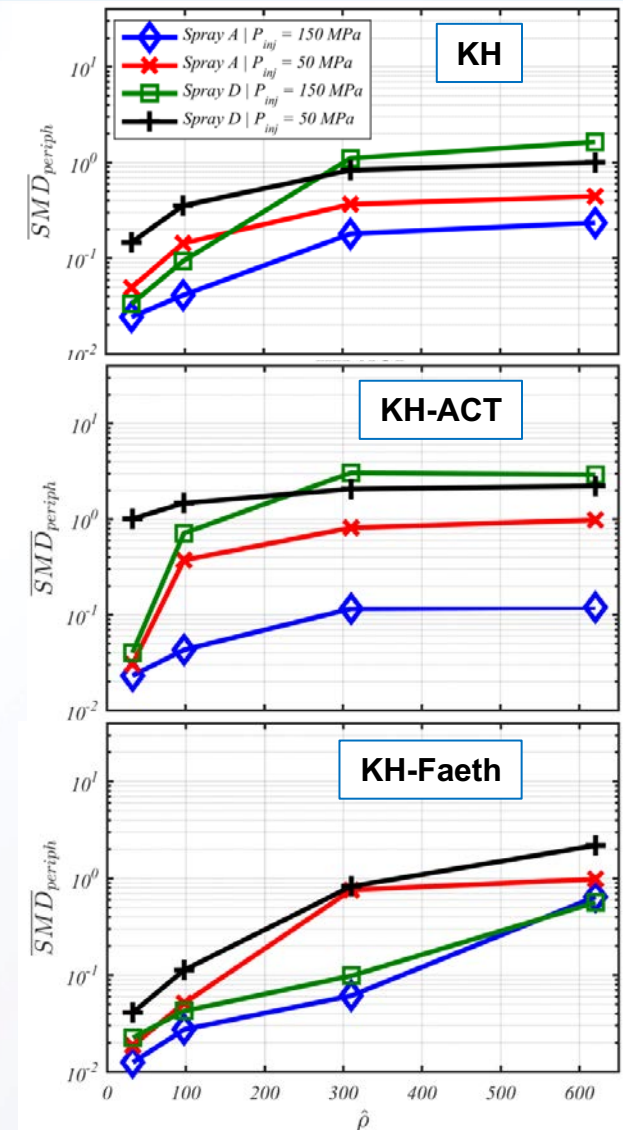
Responses to Previous Year Reviewers' Comments

- This project is a new start.

Remaining Challenges and Barriers

Spray Diagnostic Development and Experiments

- **Viable regions for application of SAMR are limited by optical thickness and radiography measurement limitations.**
  - Radiography suffers from low SNR in "wings" of spray
    - Fuels with better x-ray absorption will not have well-characterized physical and optical properties
  - Optical thickness measurements suffer from multiple scattering at spray centerline
- **SAMR uncertainties are not yet fully quantified.**
  - Uncertainties in co-alignment of radiography and optical thickness measurements
  - Spray asymmetries are more evident in "wings" of spray
    - SMD in these regions are especially sensitive to measurement co-alignment

Spray Model Development

- **Lagrangian spray models are known to exhibit grid sensitivities and this may bias conclusions.**
- **Quantitative validation data is limited from BP1 due to measurement challenges.**
  - Unable to perform full model sensitivity analysis until BP2 data complete

Proposed Future Research

## Spray Diagnostic Development and Experiments

- **BP2 Experiments**
  - Improve radiography SNR and quantify/minimize SAMR measurement uncertainties.
    - Improve SNR in radiography measurements via use of Viscor with cerium doping
    - Quantify multiple scattering errors in determination of SMD
    - Increase number of viewing angles to better understand/quantify spray asymmetries
  - Revisit select BP1 experiments with improved SAMR methodology and more viewing angles to quantify asymmetries.
  - Expand data processing – 2D maps of LVF and SMD.

Spray Model Development

- **BP2 Modeling**
  - Evaluation of benchmark spray models against available BP1 experiments to determine model improvement path (ongoing).
    - Continued evaluation of models as new quantitative data becomes available
  - Evaluate turbulent breakup correlations from Faeth et al. as new turbulent atomization modeling approach (ongoing).
  - Further examine grid and other numerical sensitivities on model predictions.

Any proposed future work is subject to change based on funding levels.

Summary
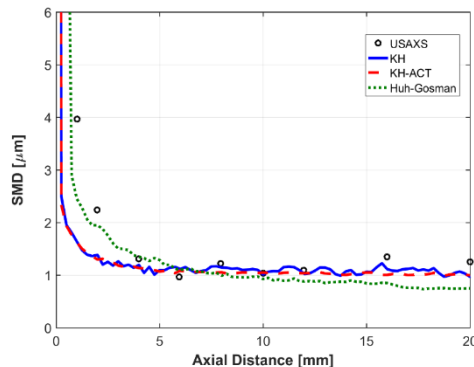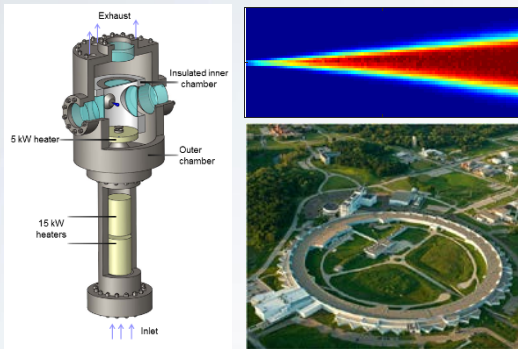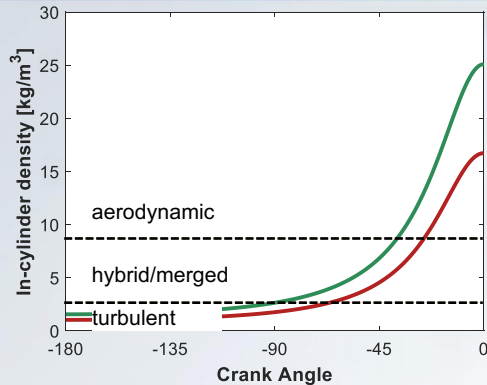
- **This project is developing a new multi-physics spray model for advanced combustion regimes.**
  - Atomization physics are different - liquid turbulence is known to control breakup at low $\rho_{ambient}$
  - Project based on a rigorous assessment of models against quantitative spray morphology measurements
- **Project addresses lack of quantitative data for spray model development and validation.**
  - Focused on generating data across a wide range of conditions relevant for advanced combustion strategies
  - Contributes to Engine Combustion Network (Spray A and D)
- **Demonstrated new collaborative measurement technique (SAMR) that quantifies 2D/3D spray morphology in practical diesel sprays.**
- **Model benchmarking and development is being conducted in OpenFOAM.**
  - Ensures open-source compatibility of delivered multi-physics spray model.
- **New turbulent atomization model appears necessary to capture correct spray breakup at low $\rho_{ambient}$**

Technical Back-Up Slides

Experimental conditions for this project are focused on turbulent/aerodynamic break-up regime transitions.
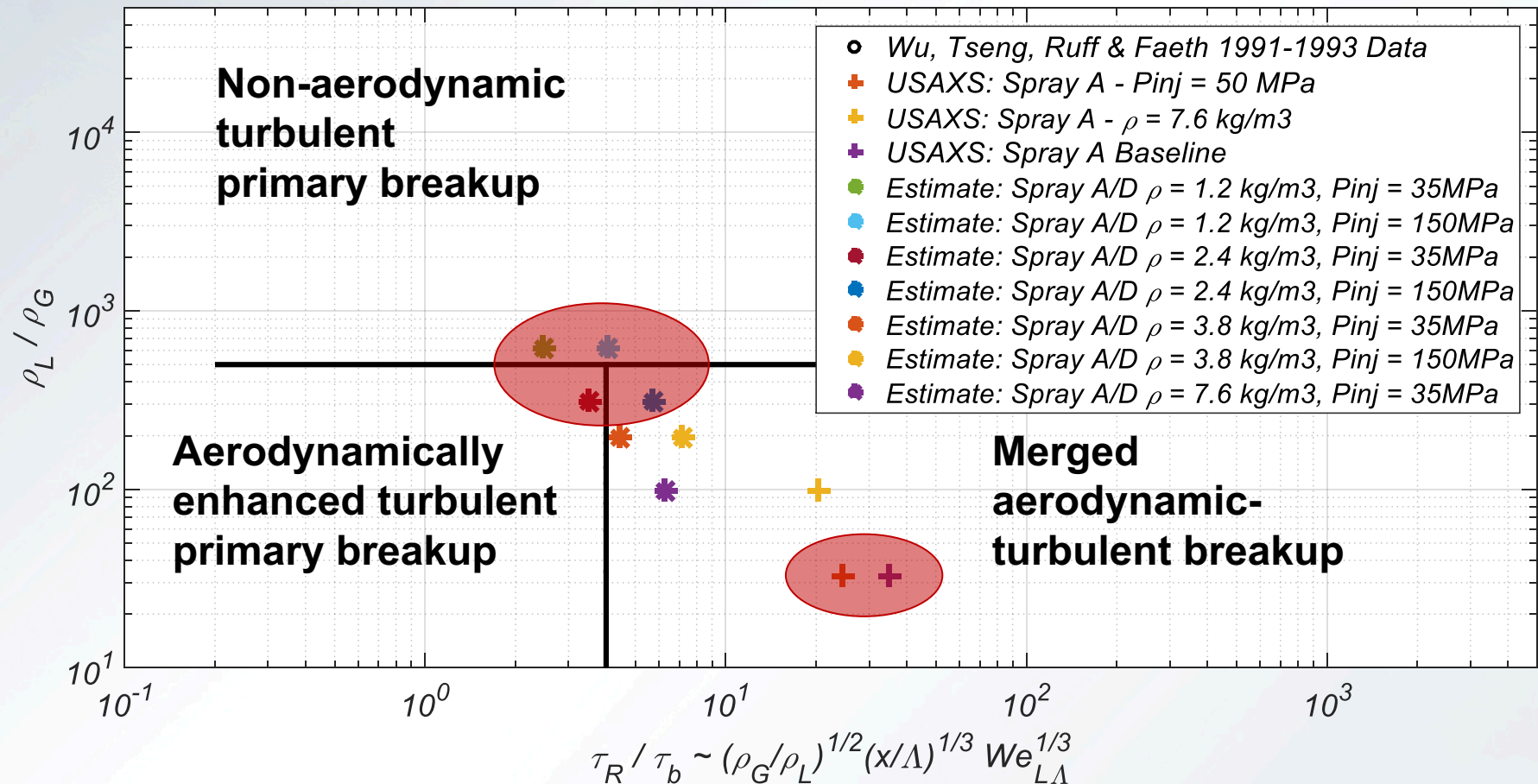
The open source software MiePlot is used to calculate droplet Mie-scattering cross sections, which are then used to quantify SMD from the Scattering-Extinction measurement.
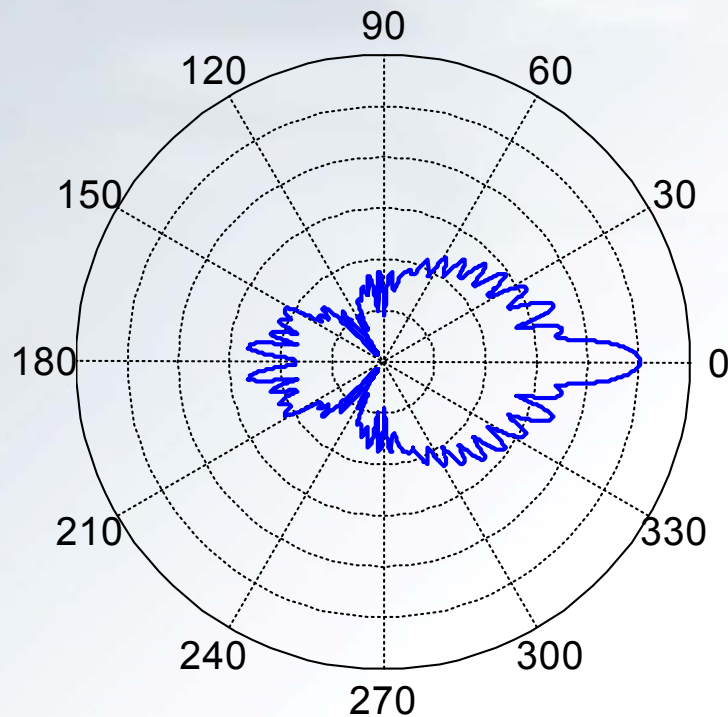
Polar scattering intensity distribution for a 5 μm dodecane droplet illumination wavelength, λ = 633 nm

633 nm
220 mrad collection angle
ref. index, n = 1.422
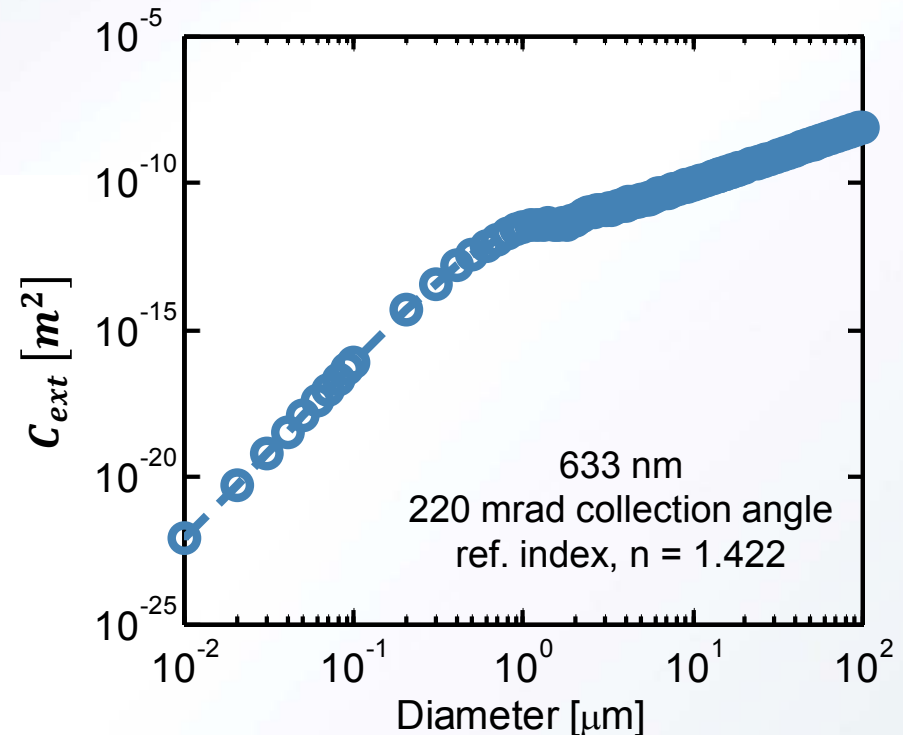
Cext is proportional to the amount of light scattered in all directions outside of the measurement collection angle

Complete test matrix of target non-vaporizing spray experimental conditions for this project.

#	ECN Nozzle Type	Ambient Density [kg/m³]	Injection Pressure [MPa]	DBI Measurements
1	Spray D	1.2	150	complete
2	Spray D	1.2	50	complete
3	Spray D	1.6	150	complete
4	Spray D	1.6	50	complete
5	Spray D	2.4	150	complete
6	Spray D	2.4	50	complete
7	Spray D	22.8	150	complete
8	Spray D	22.8	50	complete
9	Spray A	1.2	150	complete
10	Spray A	1.2	50	complete
11	Spray A	22.8	150	complete
12	Spray A	22.8	50	complete
13	Spray C	1.2	150	Not yet complete
14	Spray C	1.2	50	

Small Angle Scattering (SAXS) measures path-integrated SMD in optically thick regions of the spray.

- Measurement: count the number of scattered x-rays as a function of angle ⇨ **surface area**

- Measure **density** using radiography

- Combine surface area measurement with density measurement ⇨ **Sauter Mean Diameter**

- Expensive, but useful in regions where no other measurements can succeed